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## YOU HAVE REQUESTED DATA FROM 3 ANSWERS - CONTINUE? Y/(N):y

ANSWER 1 OF 3 CAPLUS COPYRIGHT 1997 ACS 1994:668294 CAPLUS

ACCESSION NUMBER:

121:268294

DOCUMENT NUMBER:

TITLE:

Structure and absolute configuration of a

monohydrate of calcipotriol,

(1.alpha., 3.beta., 5Z, 7E, 22E, 24S) -24-cyclopropyl-9,10-secochola-5,7,10(19),22-tetraene-1,3,24-

triol. [Erratum to document cited in

CA118(24):245113x]

AUTHOR (S):

Larsen, Sine; Hansen, Erik T.; Hoffmeyer, lene;

Rastrup-Andersen, Niels

CORPORATE SOURCE:

Dep. Chem., Univ. Copenhagen, Copenhagen,

DK-2100, Den.

SOURCE:

Acta Crystallogr., Sect. C: Cryst. Struct.

Commun. (1993), C49(12), 2184 CODEN: ACSCEE; ISSN: 0108-2701

DOCUMENT TYPE:

Journal English

LANGUAGE:

AB

The errors were reflected in the abstr.

147657-22-5

RL: PRP (Properties)

(crystal structure and abs. configuration of (Erratum))

RN 147657-22-5 CAPLUS

monohydrate, (1.alpha., 3.beta., 5Z, 7E, 22E, 24S) - (9CI) (CA INDEX

9,10-Secochola-5,7,10(19),22-tetraene-1,3,24-triol, 24-cyclopropyl-,

NAME)

Absolute stereochemistry.

Double bond geometry as shown.

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ACCESSION NUMBER: 1994:631161 CAPLUS DOCUMENT NUMBER: 121:231161 TITLE: Preparation and formulation of calcipotriol hydrate INVENTOR (S): Hansen, Erik Torngaard; Rastrup, Andersen Niels Smidt; Ringborg, Lene Hoffmeyer PATENT ASSIGNEE(S): Leo Pharmaceutical Products Ltd. a/s, Den. SOURCE: PCT Int. Appl., 10 pp. CODEN: PIXXD2 NUMBER DATE -----\_\_\_\_\_ PATENT INFORMATION: WO 9415912 A1 940721 W: AU, BB, BG, BR, BY, CA, CN, CZ, FI, HU, JP, DESIGNATED STATES: KP, KR, KZ, LK, LV, MG, MN, MW, NO, NZ, PL, RO, RU, SD, SK, UA, US, UZ, VN RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG APPLICATION INFORMATION: WO 94-DK11 940107 PRIORITY APPLN. INFO.: GB 93-763 930115 DOCUMENT TYPE: Patent LANGUAGE: English The present invention relates to calcipotriol hydrate, a new cryst. form of calcipotriol, with superior tech. properties and with superior stability. IT147657-22-5P RL: BAC (Biological activity or effector, except adverse); IMF (Industrial manufacture); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (prepn. and formulation of new crystn. form)

9,10-Secochola-5,7,10(19),22-tetraene-1,3,24-triol, 24-cyclopropyl-,

monohydrate, (1.alpha.,3.beta.,5Z,7E,22E,24S)- (9CI) (CA INDEX

Absolute stereochemistry.

Double bond geometry as shown.

147657-22-5 CAPLUS

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CN

NAME)

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L2 ANSWER 3 OF 3 CAPLUS COPYRIGHT 1997 ACS

ACCESSION NUMBER: 1993:245113 CAPLUS

DOCUMENT NUMBER: 118:245113

TITLE: Structure and absolute configuration of a

monohydrate of calcipotriol,

(1.alpha.,3.beta.,5z,7E,22E,24S)-24-cyclopropyl-9,10-secochola-5,7,10(19),22-tetraene-1,3,24-

triol

AUTHOR(S): Larsen, Sine; Hansen, Erik T.; Hoffmeyer, Lene;

Rastrup-Andersen, Niels

CORPORATE SOURCE: Dep. Chem., Univ. Copenhagen, Copenhagen,

DK-2100, Den.

SOURCE: Acta Crystallogr., Sect. C: Cryst. Struct.

Commun. (1993), C49(3), 618-21 CODEN: ACSCEE; ISSN: 0108-2701

DOCUMENT TYPE: Journal LANGUAGE: English

AB The title compd. is monoclinic, space group P21, with a 9.4377(10), b 6.9780(11), c 18.559(3) .ANG., and .beta. 93.240(13).degree.; Z = 2, dc = 1.172; R = 0.050, Rw = 0.064 for 3913 reflections. At. coordinates are given. The abs. configuration of calcipotriol was established to be 1S,3R,8R,14S,17R,20S,24S. The mol. geometry of calcipotriol is similar to the stereochem. obsd. in the structures of the related D vitamins.

IT 147657-22-5, Calcipotriol monohydrate

RL: PRP (Properties)

(crystal structure and abs. configuration of)

RN 147657-22-5 CAPLUS

CN 9,10-Secochola-5,7,10(19),22-tetraene-1,3,24-triol, 24-cyclopropyl-,
 monohydrate, (1.alpha.,3.beta.,5Z,7E,22E,24S)- (9CI) (CA INDEX
 NAME)

Absolute stereochemistry.
Double bond geometry as shown.

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(FILE 'HOME' ENTERED AT 11:58:32 ON 19 NOV 1997)

FILE 'REGISTRY' ENTERED AT 11:58:51 ON 19 NOV 1997
L1 1 S CALCIPOTRIOL MONOHYDRATE/CN

FILE 'CAPLUS' ENTERED AT 11:59:17 ON 19 NOV 1997 L2 3 S L1

FILE 'USPATFULL' ENTERED AT 12:00:13 ON 19 NOV 1997 L3 0 S L1